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OXYGEN INDUCED TRIPLET STATE TRANSITIONS OF BENZENE IN CRYOGENI--ETC(U)  
SEP 81 J LEE, E R BERNSTEIN  
N00014-79-C-0647  
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Contract <sup>15</sup> N00014-79-C-0647

<sup>14</sup> Technical Report No. 4

<sup>6</sup> OXYGEN INDUCED TRIPLET STATE TRANSITIONS OF BENZENE  
IN CRYOGENIC SOLUTIONS

by

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Prepared for Publication in  
The Journal of Chemical Physics

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<sup>11</sup> 16 September 1981

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OXYGEN INDUCED TRIPLET STATE TRANSITIONS OF BENZENE  
IN CRYOGENIC SOLUTIONS\*

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\*supported in part by grants from ONR and NSF.

# ABSTRACT

A new way of investigating the oxygen induced triplet state transitions of simple organic molecules is presented. The method involves dissolving the organic along with oxygen in hydrocarbon liquids such as propane, ethane, or propene. Both  ${}^3B_{1u} \leftarrow {}^1A_{1g}$  and  ${}^3E_{1u} \leftarrow {}^1A_{1g}$  transitions of  $C_6H_6$  and  $C_6D_6$  are studied in this work. These results indicate that both triplet states and their vibrational spacings are quite sensitive to the environment. The suggested dominant feature of the  ${}^3B_{1u}$  state of  $C_6H_6$  is  $\nu_8$  ( $916\text{ cm}^{-1}$ ) of  $e_{2g}$  symmetry. Observed triplet state intensity enhancement is believed to be due to a non-statistical oxygen/benzene van der Waals complex formed in the low temperature liquid.

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## I. INTRODUCTION

The first triplet state absorption of benzene ( $^3B_{1u} \leftarrow ^1A_{1g}$ ) has been observed in pure crystal<sup>1a,b</sup> and  $O_2$  perturbed systems.<sup>2</sup> The origin of the  $^3B_{1u}$  state has been observed around  $29,600\text{cm}^{-1}$  for both environments due to the breakdown of  $D_{6h}$  selection rules. However, the dominant series observed in the  $^3B_{1u}$  state absorption are superficially different in each environment and have thus been assigned differently. In the pure crystal the dominant series is the pseudo - Jahn Teller active  $e_{2g}$  mode  $\nu_8$  ( $240\text{cm}^{-1}$ ). In the  $O_2$  perturbed gas and matrix studies the dominant series has been assigned as the totally symmetric  $\nu_1$  ( $\sim 900\text{cm}^{-1}$ ). These apparently conflicting results and the presumed environmental sensitivity of the benzene  $^3B_{1u}$  state have sparked our interest in reinvestigating such transitions in cryogenic liquids.<sup>3</sup>

The second triplet state of benzene has been identified as the orbitally degenerate  $^3E_{1u}$  state and has been theoretically predicted to be located between the  $^3B_{1u}$  and  $^1B_{2u}$  states.<sup>4</sup> Experimental observations have been made in pure and  $O_2$ -mixed crystals; however, weak and broad features have made it impossible to analyze these data in any detail. Nonetheless, the irregular band locations of the pure and  $O_2$ -mixed system, like those for the  $^3B_{1u}$  state, make it quite clear that the Jahn Teller active  $^3E_{1u}$  state is also strongly dependent on its environment. Hence, the simultaneous observation of  $C_6H_6$  (or  $C_6D_6$ )  $^3B_{1u}$  and  $^3E_{1u}$  states in cryogenic liquids not only demonstrates a new reliable technique for the study of molecular triplet states but also serves as a direct comparison with other methods to elucidate environmental effects on triplet states.

In previous cryogenic liquid solution experiments<sup>3</sup>,  $C_6H_6$  absorption spectra of the  $^1B_{2u} \leftarrow ^1A_{1g}$  transition were studied in liquid  $N_2$ ,  $CO$ ,  $CF_4$ ,  $CH_4$ ,  $C_2H_6$ ,  $C_3H_8$  and  $NF_3$ . Three conclusions from these previous experiments are important for our present work. First, the appearance of a very weak origin (0,0)

transition indicates only a slight deviation from  $D_{6h}$  symmetry due to the presence of the cryogenic liquid. Second, the dominant vibronic series involve the  $e_{2g}$  modes  $\nu_6$  (very intense),  $\nu_8$ ,  $\nu_9$ , and  $\nu_7$ ; as is well known,  $\nu_6$  (C-C-C banding mode) effectively couples the  ${}^1B_{2u}$  and  ${}^1E_{1u}$  electronic states. Third, nonequilibrium solute aggregation occurs during low temperature deposition of cryogenic liquid solutions.<sup>3b</sup> Based on these three observations, one can anticipate that for low temperature deposition, the cryogenic liquid  $C_3H_8$  may trap the  $O_2/C_6H_6$  complex and that, like the  ${}^1B_{2u}$  state, the induced  ${}^3B_{1u}$  state absorption should possess strong vibronic origins of  $e_{2g}$  symmetry (especially  $\nu_8$ ) with possibly a much weaker solvent or complex induced origin.

## II. EXPERIMENTAL

Sample preparation and instrumental set up are described in previous reports.<sup>3</sup>  $C_6H_6$  (Fischer Gold label) and  $C_6D_6$  (Merck, Sharpe and Dohme) are further purified by vacuum distillation over potassium to remove water and other oxygen containing impurities.  $C_3H_8$  and  $O_2$  (research purity, Matheson) are further purified by distillation through cold trapped 4A molecular sieve. The absorption cell (3.8cm pathlength) is attached to a Cryodine mechanical helium refrigerator (CT1-350). Temperature of the cell can be controlled from 12K to room temperature by a Lake Shore DTC-500SP temperature controller.

Solubility of benzene in liquid  $C_3H_8$  at 87K is a critical factor in these experiments. It has previously been determined that  $C_6H_6$  ( $C_6D_6$ ) is soluble in  $C_3H_8$  to about 100 ppm at 87K. At such concentrations triplet state absorptions are, of course, not observed. It is necessary to have  $O_2$  present in the solution to enhance the triplet state transitions through the well known charge transfer mechanism. The addition of roughly 1000 ppm  $O_2$  to the solution does not affect the solubility of benzene in liquid  $C_3H_8$  as  $O_2$  is miscible with  $C_3H_8$  in this concentration range.

In the  $C_6H_6$  ( $C_6D_6$ )/ $O_2$ / $C_3H_8$  experiments, gas phase  $C_6H_6$  ( $C_6D_6$ ) and  $O_2$  are mixed in a 15ml manifold and then, together with  $C_3H_8$ , are rapidly deposited into the precooled absorption cell at 70K. Absorption spectra are taken for clear solutions at 87K.

### III. RESULTS

Figures 1 and 2 show the  $C_6H_6$  spectra of  $^3E_{1u} \leftarrow ^1A_{1g}$  and  $^3B_{1u} \leftarrow ^1A_{1g}$  transitions, respectively. Figure 3 shows the spectrum of the  $C_6D_6$   $^3E_{1u} \leftarrow ^1A_{1g}$  transition. The estimated ratio of  $C_6H_6$  ( $C_6D_6$ ): $O_2$ : $C_3H_8$  is 1:10:10<sup>4</sup>. Table I summarizes the observed frequencies. The data reported are based on many experiments whose values are averaged. For such weak features, sample to sample reproducibility and the simultaneous observation of both triplet states are important factors in the confidence level of the assignments.

In order to insure that the observed spectra are due to the  $O_2$  induced triplet state transitions of benzene, the following experiments have been carried out. Two component experiments, at the same concentrations as the three component experiments, show that in order to observe these tabulated features, all three components must be present. Moreover, in the 2600 Å region the (very weak broad)  $O_2$  Herzberg bands are observed but they do not coincide with the  $^3E_{1u} \leftarrow ^1A_{1g}$  assigned features. In the three component system, the Herzberg bands are not observed, as the  $^1B_{2u} \leftarrow ^1A_{1g}$   $C_6H_6$  transition overlaps them to some extent but also because the  $O_2$ - $O_2$  pairs are probably more weakly bound than the  $C_6H_6/O_2$  complex. No  $O_2$  related features appear in the  $^3B_{1u} \leftarrow ^1A_{1g}$  region.



## IV. DISCUSSION

Table II gives a comparison of the  ${}^3E_{1u} \leftarrow {}^1A_{1g}$  absorption features of  $O_2/C_6H_6$  ( $C_6D_6$ )/ $C_3H_8$ , the pure crystal, and other  $O_2$ -perturbed systems. Variation of band positions among these three data sets may be due to a large environmental sensitivity displayed by the Jahn Teller active  ${}^1E_{1u}$  system. The origin of the  ${}^3E_{1u}$  state has not been positively identified, either in this or in previous work. However, since an  $E_{1u} \leftarrow A_{1g}$  transition is dipole allowed in  $D_{6h}$  symmetry and  $e_{2g}$  modes are Jahn Teller active in  $E_{1u}$ , one can surmise that the first feature is the origin and the second one is the first quantum of  $\nu_6$  (or possible  $\nu_8$ ).

The  ${}^3B_{1u} \leftarrow {}^1A_{1g}$  transition of  $C_6H_6$  ( $C_6D_6$ ) has been studied in the  $O_2$ -perturbed gas phase and matrix environments, and in the pure crystal. A weak origin has been observed and assigned in these systems. However, the dominant series for the  $O_2$ -perturbed and crystal spectra have been treated in quite a different manner.

In the pure crystal system the intense absorption series involve the  $e_{2g}$  modes  $\nu_8$ ,  $\nu_6$ , and  $\nu_9$  with the major feature  $\nu_8$  (CH stretching) assigned a frequency of  $240\text{cm}^{-1}$ . Theoretical calculations confirm that the effective vibronic coupling between  ${}^3B_{1u}$  and  ${}^3E_{1u}$  is via the  $\nu_8$  mode and conclude that  $\nu_8$  may have its frequency depressed considerable in the presence of this strong pseudo Jahn Teller or Herzberg Teller coupling. Moreover, phosphorescence data from  $C_6H_6/C_6D_6$  mixed crystals<sup>6</sup> also indicate the dominant nature of  $\nu_8$  for the  ${}^3B_{1u}$  state intensity.

For the  $O_2$ -perturbed systems, on the other hand, the observed  $\sim 900\text{cm}^{-1}$  progression built on the origin has been previously assigned to be a  $\nu_1$  ( $a_{1g}$ ) series. This assignment is based solely on the idea that a  $900\text{cm}^{-1}$  mode is close to the ground state and  ${}^1B_{2u}$  state value for  $\nu_1$ . The presence of  $O_2$  has been assumed to lower the  $D_{6h}$  symmetry of  $C_6H_6$  ( $C_6D_6$ ) to probably  $D_{2h}$ , rendering the totally symmetric origin progression allowed. However, this

scheme ignores two points: 1) it is unlikely that the  $\nu_8$  progression, even in this lowered symmetry system, would disappear; and 2) the  $\sim 900\text{cm}^{-1}$  progression is highly irregular.<sup>2</sup>

From the above argument, it would seem that in the presence of  $\text{O}_2$ , the  $^3\text{B}_{1\text{u}}$  state of benzene loses its  $\text{D}_{6\text{h}}$  character completely. This, however, does not appear to be the case in the cryogenic liquid  $\text{O}_2$ -perturbed systems. First, the same  $^1\text{B}_{2\text{u}} + ^1\text{A}_{1\text{g}}$  spectra are observed with or without even large amounts ( $10^3$  ppm) of  $\text{O}_2$  in the propane. This implies that  $\text{D}_{6\text{h}}$  symmetry still holds for  $\text{C}_6\text{H}_6$  even in the  $\text{O}_2/\text{C}_6\text{H}_6$  complex. Second, neither the origin nor a  $\sim 900\text{cm}^{-1}$  progression has been identified in the present study. This negative evidence calls into question the nature of the  $900\text{cm}^{-1}$  series observed in the gas and matrix  $\text{O}_2$ -perturbed investigations. The most probable explanation for these data is that the band at  $(0,0) + 900\text{cm}^{-1}$  is  $\nu_8$  and the irregular series built on this is  $8_0^n$  or  $8_0^1 1_0^n$  as given by the elegant crystal results. In this reinterpretation, the presence of  $\text{O}_2$ , instead of destroying the  $\text{D}_{6\text{h}}$  nature of the  $^3\text{B}_{1\text{u}}$  state, at most shifts the frequency of  $\nu_8$  from  $1450\text{cm}^{-1}$  ( $^1\text{B}_{2\text{u}}$ ) to roughly  $900\text{cm}^{-1}$  in the  $^3\text{B}_{1\text{u}}$  state. Moreover, a good deal of this frequency shift is probably attributable to the pseudo Jahn Teller or Herzberg Teller coupling between the  $^3\text{B}_{1\text{u}}$  and  $^3\text{E}_{1\text{u}}$  states induced by  $\nu_8$ . The  $\text{O}_2$ -perturbed data are compared to each other and the crystal data in Table III.

If the  $^3\text{B}_{1\text{u}}$  crystal origin is assumed to be similar in energy to the unobserved  $\text{O}_2/\text{C}_3\text{H}_8$  liquid perturbed  $^3\text{B}_{1\text{u}}$  origin (gas to liquid and gas to crystal shifts are quite similar for  $\text{C}_6\text{H}_6^3$ ), then a value of  $916\text{cm}^{-1}$  for  $\nu_8$  can be obtained. The large difference between the pseudo Jahn Teller  $\nu_8$  frequency in the crystal and  $\text{O}_2$ -perturbed systems may be an environmental effect. The second band, located  $567\text{cm}^{-1}$  above the first, could be either  $8_0^2$  or  $8_0^1 6_0^1$ . A concrete determination is not possible with the present data.

Perhaps the most interesting and significant aspect of the present experiments has to do with the  $O_2/C_6H_6/C_3H_8$  system itself. In these dilute cryogenic solutions,  $C_6H_6:O_2:C_3H_8 = 1:10:10^4$ , the statistical probability for  $O_2/C_6H_6$  pair formation is of the order of  $10^{-7}$ . Such a low concentration of (statistical) pairs could not possibly be responsible for the observed absorptions. It seems certain that there must be a preferential  $O_2/C_6H_6$  interaction and that this interaction results in a decidedly non-statistical  $O_2/C_6H_6$  "pair" formation. These pairs or clusters may be regarded as "van der Waals" molecules or clusters. We are presently studying the properties of these interesting systems in order to elucidate cluster size (1 to 1  $O_2/C_6H_6$  or n to 1  $O_2/C_6H_6$ ), cluster life time, cluster photochemistry, and other cluster excited and ground states. The nature of the  $O_2/C_6H_6$  potential interaction in cryogenic liquid should prove important in the understanding of the recently reported aggregation phenomena in cryogenic liquids.<sup>3b</sup>

## V. CONCLUSIONS

The observation of  $O_2$ -induced triplet transition intensity in cryogenic liquid solutions represents yet another application of such systems to the study of molecular, aggregation, and liquid state phenomena. Moreover, such mixed cryogenic liquids can provide a new data set with which to analyze the triplet states of organic molecules. In the  $C_6H_6$  ( $C_6D_6$ )/ $O_2$ / $C_3H_8$  system, as an example, three conclusions can be reached.

1.  $\nu_8$  ( $e_{2g}$ ) effectively couples the  $^3B_{1u}$  and  $^3E_{1u}$  states and appears to dominate the  $^3B_{1u} \leftarrow ^1A_{1g}$  absorption spectrum in all environments.
2.  $\nu_8$  in the  $^3B_{1u}$  state is quite sensitive to environmental perturbations: in  $O_2$ -perturbed systems its value is  $\sim 900\text{cm}^{-1}$  but in the crystal its value is  $\sim 250\text{cm}^{-1}$ .
3.  $C_6H_6$  triplet state energies, in general, both  $^3B_{1u}$  and  $^3E_{1u}$ , are sensitive to their surroundings probably because of the Jahn Teller and pseudo Jahn Teller nature of these states.

The overall triplet state intensity enhancement for  $C_6H_6$  is associated with the formation of a van der Waals complex or molecular species in the cryogenic liquid.

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TABLE I  
OBSERVED TRIPLET STATE TRANSITIONS OF  $C_6H_6$  AND  $C_6D_6$   
IN  $O_2/C_3H_8$  SOLUTIONS AT 87K.

Molecules	$C_6H_6$ ( $cm^{-1}$ )		$C_6D_6$ ( $cm^{-1}$ )	
	Frequency	Difference	Frequency	Difference
${}^3E_{1u} + {}^1A_{1g}$	36968		37067	
		587		629
	37555		37696	
${}^3B_{1u} + {}^1A_{1g}$	(29647)*			
		916		
	30563			
		562		
	31125			

\*ref. 1a: crystal result, see text for explanation.

TABLE II  
COMPARISON OF  ${}^3E_{1u}$   ${}^1A_{1g}$  DATA FOR  $C_6H_6$  AND  $C_6D_6$

Molecules	Systems		$O_2$ -Perturbed ( $cm^{-1}$ )				Crystal <sup>(2)</sup> ( $cm^{-1}$ )	
			$O_2/C_6H_6$ (1)		$O_2$ Matrix (2)			
			Frequency	Difference	Frequency	Difference		
$C_6H_6$			36968		36560		36947	
				587		610		549
			37555		37170		37496	
$C_6D_6$			37067		36784		37147	
				629		712		
			37696		37496		---	

(1) this work

(2) ref. 2b

TABLE III  
COMPARISON OF  ${}^3B_{1u} + {}^1A_{1g}$  DATA FOR  $C_6H_6$

Pure Crystal <sup>(1)</sup>		$O_2$ -Perturbed System			
Frequency( $cm^{-1}$ )	Assignments	Frequency ( $cm^{-1}$ )			New Assignments
		Cryogenic Liquid <sup>(2)</sup>	Gas Phase <sup>(3)</sup>	Matrix <sup>(4)</sup>	
29647	(0,0)	---	29516	29410	(0,0)
29886	$8_0^1$	30563	30500	30395	$8_0^1$
---	---	31125	---	---	$8_0^2$ or $8_0^6$
30787	$8_0^1$	---	31300	31350	$8_0^1$

- (1) ref. 1a
- (2) this work
- (3) ref. 2a
- (4) ref. 2c



## FIGURE CAPTIONS

### Figure 1

${}^3E_{1u} \leftarrow {}^1A_{1g}$  absorption of  $C_6H_6$  in  $O_2$  and  $C_3H_8$  mixed solution at  $87^\circ K$  (1:10:10<sup>4</sup>). The features at 2642Å and 2608Å are the (0,0) and the 6<sub>0</sub><sup>1</sup> of the  ${}^1B_{2u} \leftarrow {}^1A_{1g}$  transition of  $C_6H_6$ .

### Figure 2

${}^3B_{1u} \leftarrow {}^1A_{1g}$  absorption of  $C_6H_6$  in  $O_2$  and  $C_3H_8$  mixed solution at  $87^\circ K$  (1:10:10<sup>4</sup>).

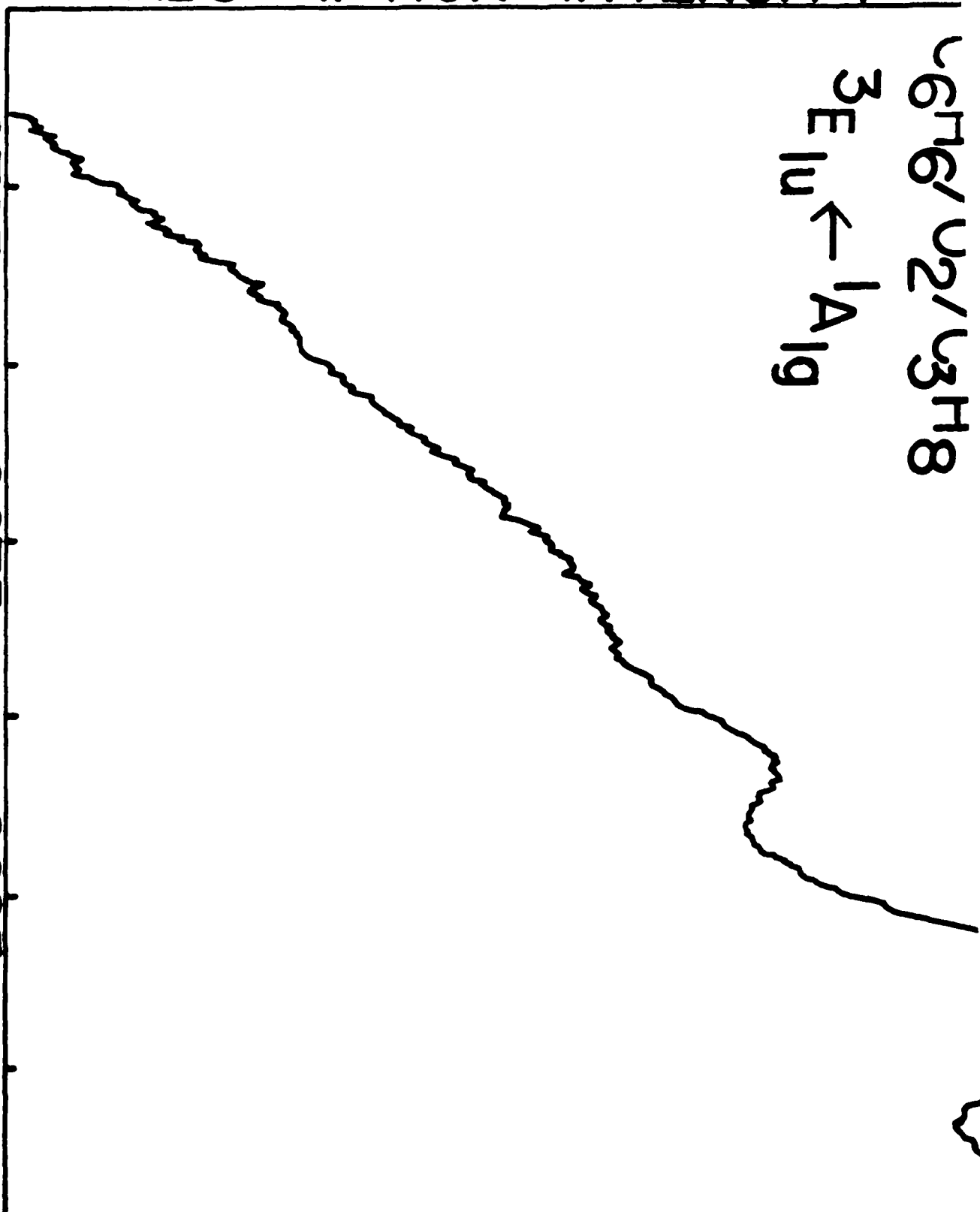
### Figure 3

${}^3E_{1u} \leftarrow {}^1A_{1g}$  absorption of  $C_6D_6$  in  $O_2$  and  $C_3H_8$  mixed solution at  $87^\circ K$  (1:10:10<sup>4</sup>). The feature at 2630Å is the (0,0) of the  ${}^1B_{2u} \leftarrow {}^1A_{1g}$  transition  $C_6D_6$ .

ABSORPTION INTENSITY

$u_2/u_3H_8$   
 $3E_{1u} \leftarrow 1A_{1g}$

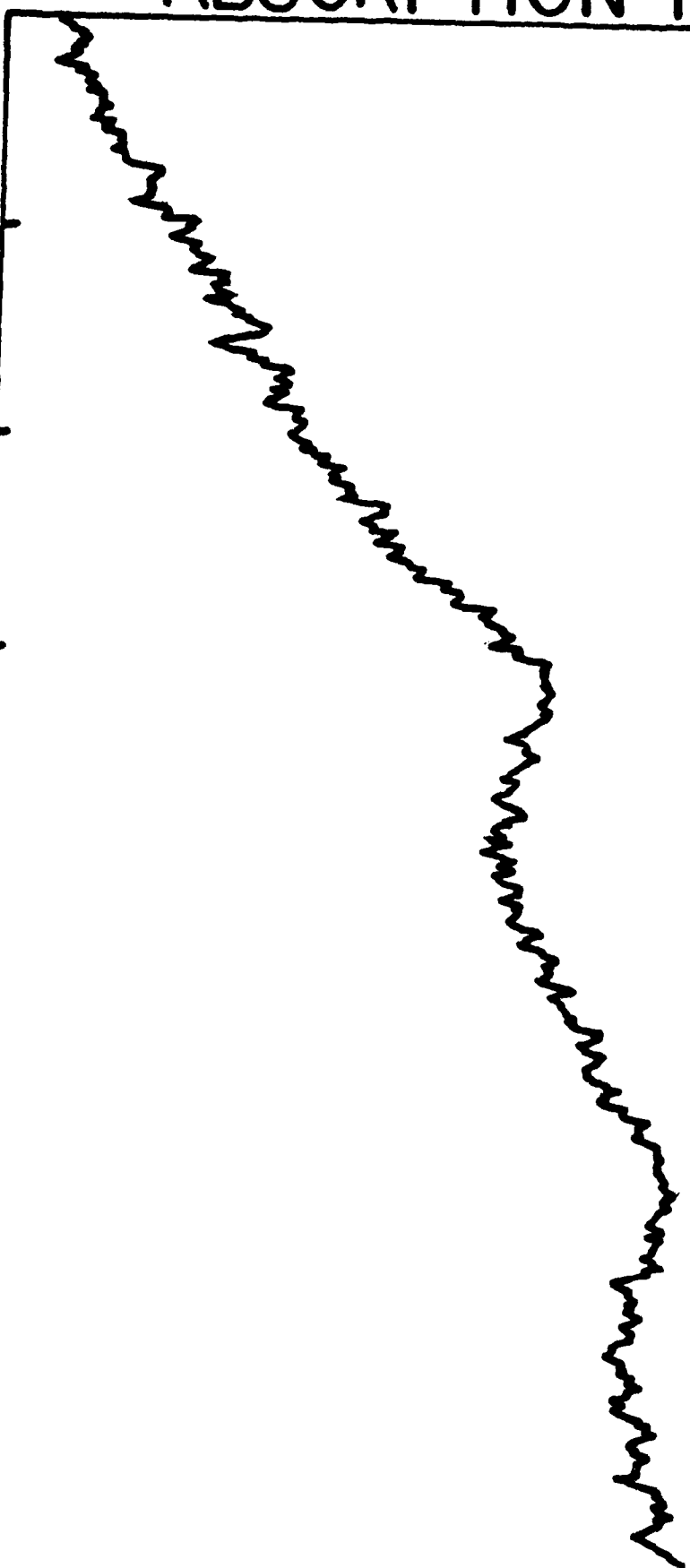
2725 2675 2625  
WAVELENGTH (Å)



u6H6/U2/C3H8

$^3B_{1u} \leftarrow ^1A_{1g}$

ABSORPTION INTENSITY



3325

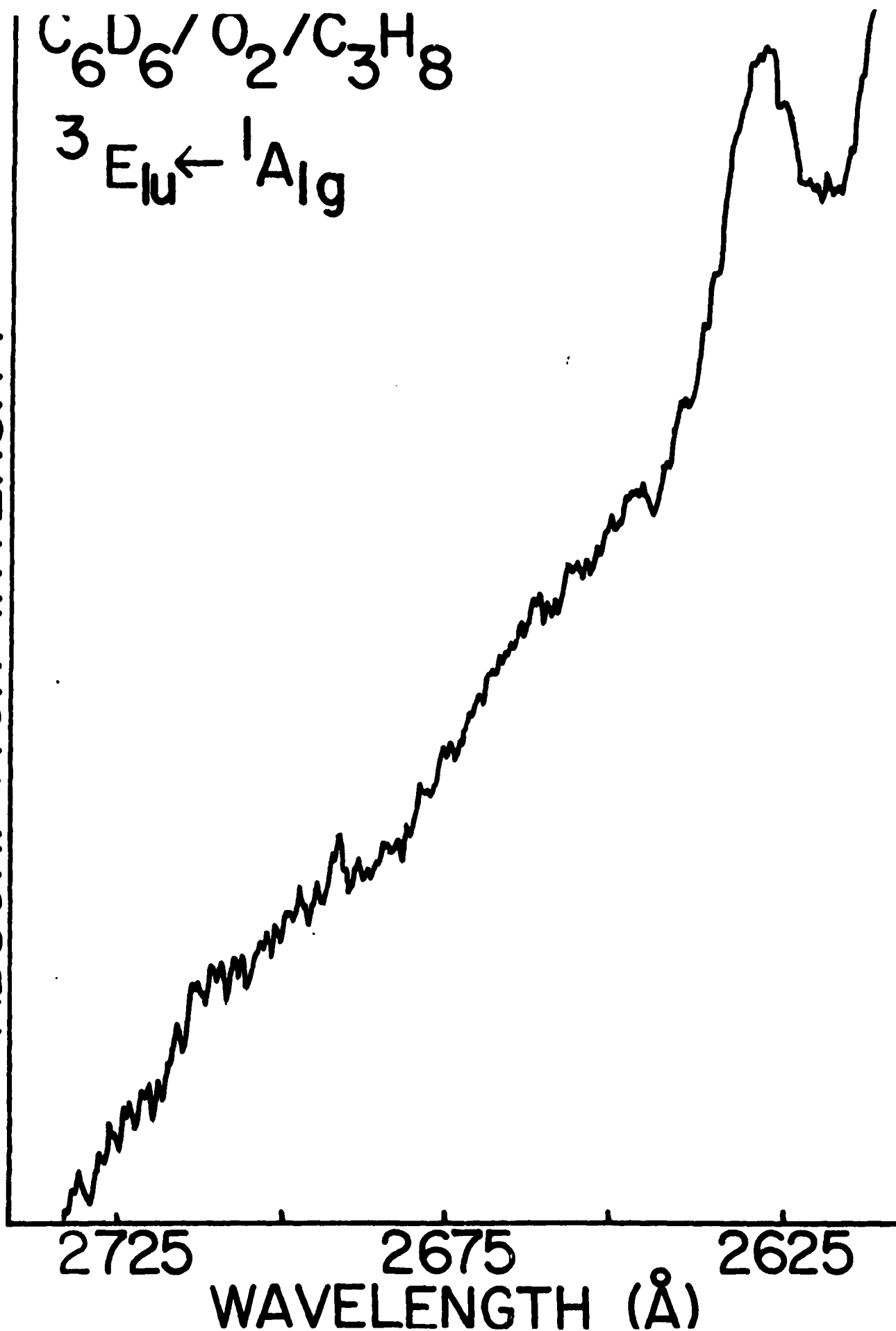
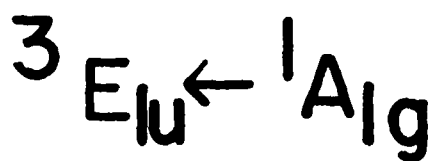
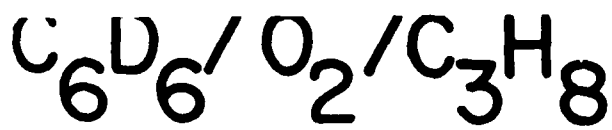
3275

3225

3175

WAVELENGTH (Å)

ABSORPTION INTENSITY



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